

Fig. 1

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The Principle of Ligand Identification

The Process

Dictionary of Interfaces in Proteins

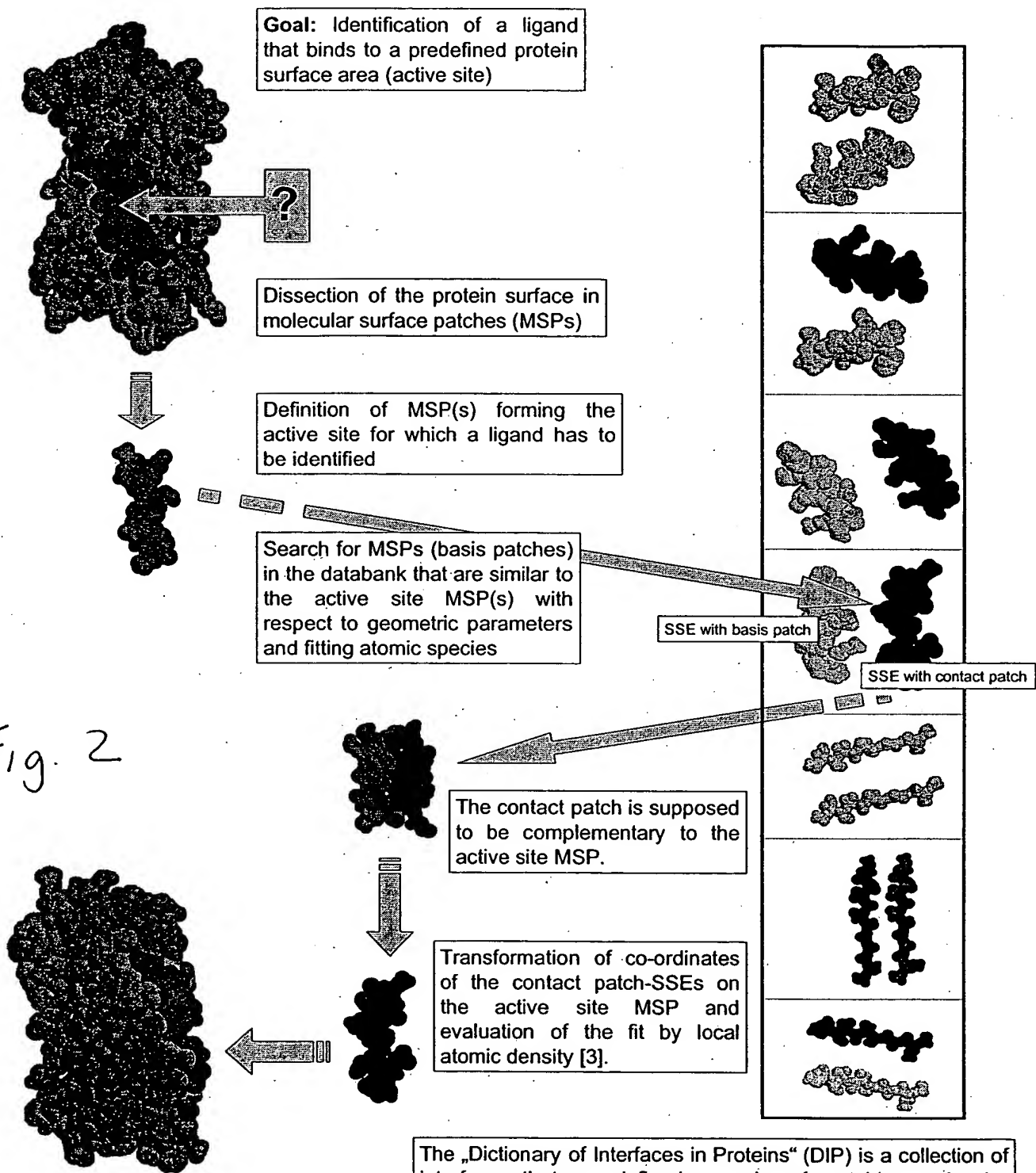


Fig. 2

Abbreviations:
SSE: secondary structural element
MSP: molecular surface patch

The „Dictionary of Interfaces in Proteins“ (DIP) is a collection of interfaces that are defined as pairs of matching molecular surface patches between neighboring secondary structural elements. Each interface consists of two subsets of atoms from neighbouring secondary structure elements (pairs of complementary MSPs). All such interfaces from known protein structures were collected in a comprehensive data bank (DIP).